

**TITLE:** USING FOURIER COEFFICIENTS FROM NEAR INFRARED SPECTRA TO  
ESTIMATE CHEMICAL CONSTITUENTS IN TOBACCO

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**ABSTRACT:** A study of the NIR spectra of 200 flue-cured tobacco samples shows that the first 11 Fourier coefficients of modeled spectra can be used to measure chemical composition. A subset of 100 samples were used to calibrate a computerized spectrophotometer. The calibrated system was then used to "predict" the composition of the other 100 samples.  $R^2$  of the calibration and standard errors of prediction (SEP) were as follows ( $R^2$ /SEP): nicotine - 0.961/0.236; nitrogen - 0.916/0.132; sugars - 0.975/0.936; water soluble nitrogen - 0.820/0.54; calcium - 0.956/0.191; potassium - 0.896/0.228. Advantages over previous NIR methods include (1) reproduction of the original spectra with as few as 50 pairs of Fourier coefficients, (2) filtering of noise without the loss of end points of the spectra, (3) reduction of storage requirements by 1/7.

**REVIEW:** In this paper the advantages of operating in the Fourier domain relative to the wavelength domain for near infrared spectra were discussed. Working in the wavelength domain requires the acquisition of approximately 1700 data points to adequately describe the sample spectra. In this mode a computation time of several hours is required in order to obtain the correlations for the various components of interest. Also the storage requirements for this large volume of spectral data points places severe strains on the computer system.

Working in the Fourier domain allows the use of only 100 Fourier coefficients to adequately describe the spectra. A subset of 11 coefficients can be used to adequately model the principal components in the sample. The first coefficient relates to the same particle size, thus using coefficients 2-12 removes the particle size parameter. Working with only 11 coefficients reduces the run time to only a few minutes and the storage allocation is reduced by 97%. This increase in processing speed and reduction in storage space allows one to run more calibration spectra, thus reducing to a minimum the standard errors of prediction for the chemical components present.

Also of interest in this paper was the ability to obtain data on potassium and calcium in tobacco even though they do not have near infrared absorption bands. This is achieved due to their association with organic molecules in the tobacco matrix.

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